Lecture 6: Clustering

Information Retrieval
Computer Science Tripos Part II

Simone Teufel

Natural Language and Information Processing (NLIP) Group

UNIVERSITY OF CAMBRIDGE

Simone.Teufel@cl.cam.ac.uk

Lent 2014

Overview

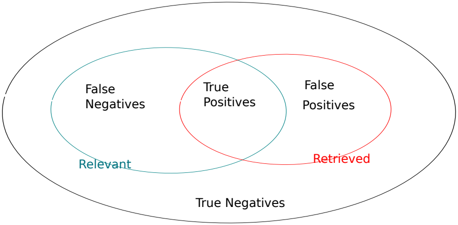
1. Recap/Catchup
2. Clustering: Introduction
3. Non-hierarchical clustering
4. Hierarchical clustering

Precision and recall

THE TRUTH

WHAT THE SYSTEM THINKS

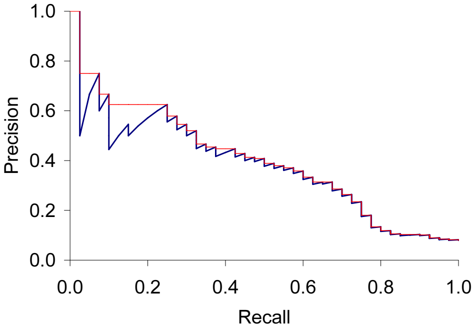
	Relevant	Nonrelevant
Retrieved	true positives (TP)	false positives (FP)
Not retrieved	false negatives (FN)	true negatives (TN)



$$\begin{aligned} P &= TP/(TP+FP) \\ R &= TP/(TP+FN) \end{aligned}$$

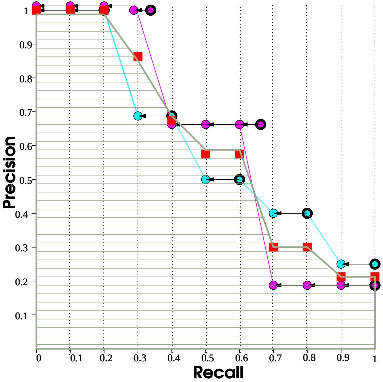
Precision/Recall Graph

Rank	Doc
1	d_{12}
2	d_{123}
3	d_4
4	d_{57}
5	d_{157}
6	d_{222}
7	d_{24}
8	d_{26}
9	d_{77}
10	d_{90}



Avg 11pt prec – area under normalised P/R graph

$$P_{11\_pt} = \frac{1}{11} \sum_{j=0}^{10} \frac{1}{N} \sum_{i=1}^{N} \tilde{P}_i(r_j)$$



Mean Average Precision (MAP)

$$MAP = \frac{1}{N} \sum_{j=1}^{N} \frac{1}{Q_j} \sum_{i=1}^{Q_j} P(doc_i)$$

Query 1		
Rank		$P(doc_i)$
1	X	1.00
2		
3	X	0.67
4		
5		
6	X	0.50
7		
8		
9		
10	X	0.40
11		
12		
13		
14		
15		
16		
17		
18		
19		
20	X	0.25
AVG:		0.564

Query 2		
Rank		$P(doc_i)$
1	X	1.00
2		
3	X	0.67
4		
5		
6		
7		
8		
9		
10		
11		
12		
13		
14		
15	X	0.2
AVG:		0.623

$$MAP = \frac{0.564+0.623}{2} = 0.594$$

What we need for a benchmark

- A collection of documents
  - Documents must be representative of the documents we expect to see in reality.
  - There must be many documents.
  - 1398 abstracts (as in Cranfield experiment) no longer sufficient to model modern retrieval
- A collection of information needs
  - ...which we will often incorrectly refer to as queries
  - Information needs must be representative of the information needs we expect to see in reality.
- Human relevance assessments
  - We need to hire/pay "judges" or assessors to do this.
  - Expensive, time-consuming
  - Judges must be representative of the users we expect to see in reality.

Second-generation relevance benchmark: TREC

- TREC = Text Retrieval Conference (TREC)
- Organized by the U.S. National Institute of Standards and Technology (NIST)
- TREC is actually a set of several different relevance benchmarks.
- Best known: TREC Ad Hoc, used for first 8 TREC evaluations between 1992 and 1999
- 1.89 million documents, mainly newswire articles, 450 information needs
- No exhaustive relevance judgments – too expensive
- Rather, NIST assessors' relevance judgments are available only for the documents that were among the top *k* returned for some system which was entered in the TREC evaluation for which the information need was developed.

Sample TREC Query

<num> Number: 508

<title> hair loss is a symptom of what diseases

<desc> Description:

Find diseases for which hair loss is a symptom.

<narr> Narrative:

A document is relevant if it positively connects the loss of head hair in humans with a specific disease. In this context, “thinning hair” and “hair loss” are synonymous. Loss of body and/or facial hair is irrelevant, as is hair loss caused by drug therapy.

TREC Relevance Judgements

Text REtrieval Conference (TREC)

Humans decide which document–query pairs are relevant.

Interjudge agreement at TREC

information need	number of docs judged	disagreements
51	211	6
62	400	157
67	400	68
95	400	110
127	400	106

- Observation: Judges disagree a lot.
- This means a large impact on absolute performance numbers of each system
- But virtually no impact on ranking of systems
- So, the results of information retrieval experiments of this kind can reliably tell us whether system A is better than system B.
- even if judges disagree.

Example of more recent benchmark: ClueWeb09

- 1 billion web pages
- 25 terabytes (compressed: 5 terabyte)
- Collected January/February 2009
- 10 languages
- Unique URLs: 4,780,950,903 (325 GB uncompressed, 105 GB compressed)
- Total Outlinks: 7,944,351,835 (71 GB uncompressed, 24 GB compressed)

Evaluation at large search engines

- Recall is difficult to measure on the web
- Search engines often use precision at top k, e.g., $k = 10$ . . .
- . . . or use measures that reward you more for getting rank 1 right than for getting rank 10 right.
- Search engines also use non-relevance-based measures.
  - Example 1: clickthrough on first result
  - Not very reliable if you look at a single clickthrough (you may realize after clicking that the summary was misleading and the document is nonrelevant) . . .
  - . . . but pretty reliable in the aggregate.
  - Example 2: A/B testing

A/B testing

- Purpose: Test a single innovation
- Prerequisite: You have a large search engine up and running.
- Have most users use old system
- Divert a small proportion of traffic (e.g., 1%) to the new system that includes the innovation
- Evaluate with an "automatic" measure like clickthrough on first result
- Now we can directly see if the innovation does improve user happiness.
- Probably the evaluation methodology that large search engines trust most

Reading

- MRS, Chapter 8

Upcoming

- What is clustering?
- Applications of clustering in information retrieval
- *K*-means algorithm
- Introduction to hierarchical clustering
- Single-link and complete-link clustering

Overview

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Clustering: Definition

- (Document) clustering is the process of grouping a set of documents into clusters of similar documents.
    - Documents within a cluster should be similar.
    - Documents from different clusters should be dissimilar.
- Clustering is the most common form of unsupervised learning.
- Unsupervised = there are no labeled or annotated data.

Difference clustering–classification

Classification	Clustering
supervised learning	unsupervised learning
classes are human-defined and part of the input to the learning algorithm	Clusters are inferred from the data without human input.
output = membership in class only	Output = membership in class + distance from centroid ("degree of cluster membership")

The cluster hypothesis

Cluster hypothesis.

Documents in the same cluster behave similarly with respect to relevance to information needs.

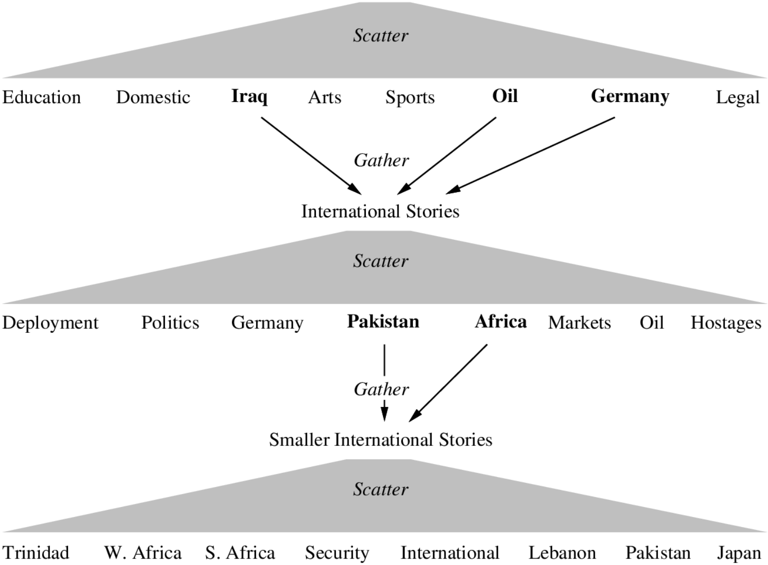
All applications of clustering in IR are based (directly or indirectly) on the cluster hypothesis.

Van Rijsbergen's original wording (1979): "closely associated documents tend to be relevant to the same requests".

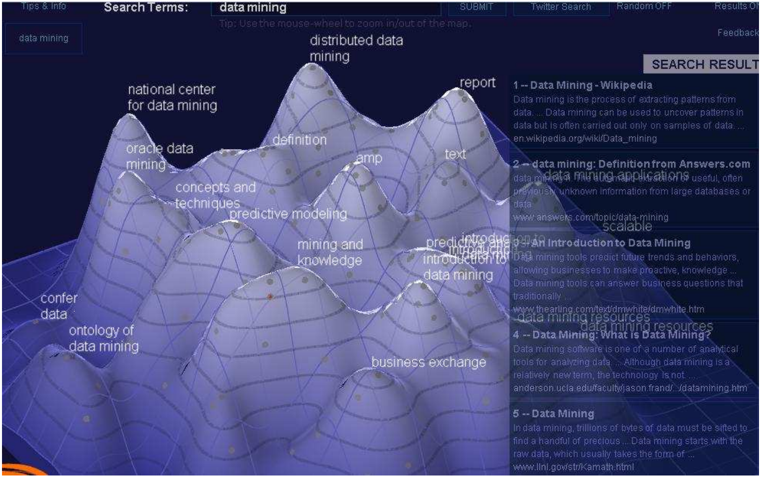
Applications of Clustering

- IR: presentation of results (clustering of documents)
- Summarisation:
  - clustering of similar documents for multi-document summarisation
  - clustering of similar sentences for re-generation of sentences
- Topic Segmentation: clustering of similar paragraphs (adjacent or non-adjacent) for detection of topic structure/importance
- Lexical semantics: clustering of words by cooccurrence patterns

Scatter-Gather



Clustering search results



1 -- Data Mining - Wikipedia
Data mining is the process of extracting patterns from data. ... Data mining can be used to uncover patterns in data but is often carried out only on samples of data. ...
en.wikipedia.org/wiki/Data_mining

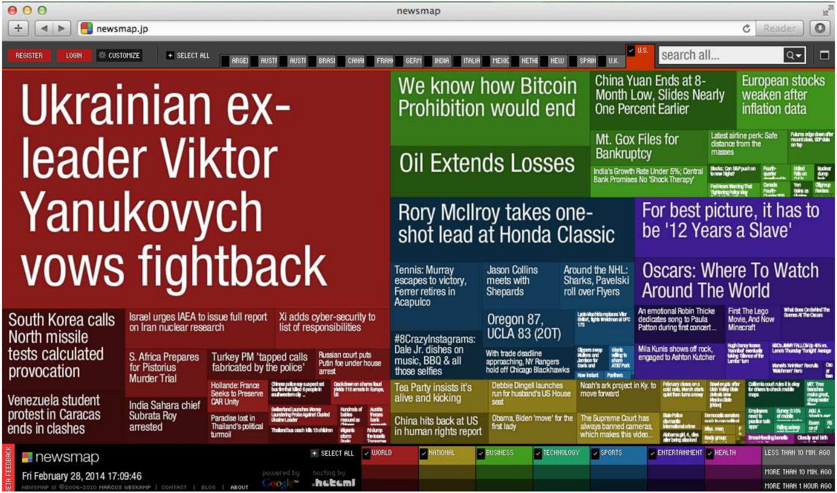
2 -- data mining: Definition from Answers.com
data mining n. The automatic extraction of useful, often previously unknown information from large databases or data
www.answers.com/topic/data-mining

3 -- An Introduction to Data Mining
Data mining tools predict future trends and behaviors, allowing businesses to make proactive, knowledge ... Data mining tools can answer business questions that traditionally ...
www.thearling.com/text/dmwhite/dmwhite.htm

4 -- Data Mining: What is Data Mining?
Data mining software is one of a number of analytical tools for analyzing data. ... Although data mining is a relatively new term, the technology is not ...
anderson.ucla.edu/faculty/jason.frand/.../datamining.htm

5 -- Data Mining
In data mining, trillions of bytes of data must be sifted to find a handful of precious ... Data mining starts with the raw data, which usually takes the form of ...
www.llnl.gov/str/Kamath.html

Clustering news articles



newsmap

newsmap.jp

Ukrainian ex-leader Viktor Yanukovych vows fightback

We know how Bitcoin Prohibition would end

Oil Extends Losses

China Yuan Ends at 8-Month Low, Slides Nearly One Percent Earlier

European stocks weaken after inflation data

Mt. Gox Files for Bankruptcy

Latest airline perk: Safe distance from the masses

Futures edge down after record close, GDP data on tap

India's Growth Rate Under 5%; Central Bank Promises No 'Shock Therapy'

Stocks: Can S&P push on to new highs?

Fed Hears Warning That Tightening Policy May

Rory McIlroy takes one-shot lead at Honda Classic

For best picture, it has to be '12 Years a Slave'

Tennis: Murray escapes to victory, Ferrer retires in Acapulco

Jason Collins meets with Shepards

Around the NHL: Sharks, Pavelski roll over Flyers

Oscars: Where To Watch Around The World

South Korea calls North missile tests calculated provocation

Israel urges IAEA to issue full report on Iran nuclear research

Xi adds cyber-security to list of responsibilities

#8CrazyInstagrams: Dale Jr. dishes on music, BBQ & all those selfies

Oregon 87, UCLA 83 (2OT)

Lyoto Machida replaces Vitor Belfort, fights Weidman at UFC 173

An emotional Robin Thicke dedicates song to Paula Patton during first concert ...

First The Lego Movie, And Now Minecraft

What Goes On Behind The Scenes At The Oscars

With trade deadline approaching, NY Rangers hold off Chicago Blackhawks

Mila Kunis shows off rock, engaged to Ashton Kutcher

Hugh Dancy teases 'Hannibal' eventually taking 'Silence of the Lambs' turn

NBC's JIMMY FALLON Up 40% vs. Leno's Thursday 'Tonight' Average

Marvel's 'Ant-Man' Recruits 'Watchmen' Hero

S. Africa Prepares for Pistorius Murder Trial

Turkey PM 'tapped calls fabricated by the police'

Russian court puts Putin foe under house arrest

Venezuela student protest in Caracas ends in clashes

India Sahara chief Subrata Roy arrested

Hollande: France Seeks to Preserve CAR Unity

Chinese police say suspect set bus fire that killed 6 people in southwestern city ...

Crackdown on shares fraud yields 110 arrests in Europe, US

Switzerland Launches Money Laundering Probe Against Ousted Ukraine Leader

Paradise lost in Thailand's political turmoil

Thailand bus crash kills 13 children

Tea Party insists it's alive and kicking

Debbie Dingell launches run for husband's US House seat

Noah's ark project in Ky. to move forward

February closes on a cold note, March starts quiet then turns snowy

California court rules it is okay for drivers to check mobile maps

China hits back at US in human rights report

Obama, Biden 'move' for the first lady

The Supreme Court has always banned cameras, which makes this video...

Alabama girl, 4, dies after being attacked

Breast-feeding benefits

Obesity and birth

Fri February 28, 2014 17:09:46

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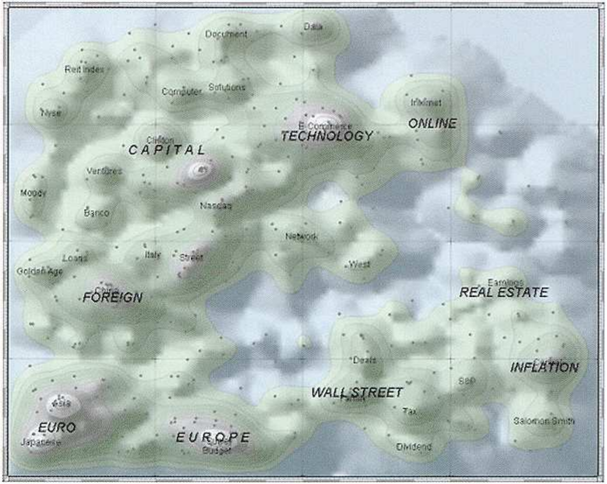
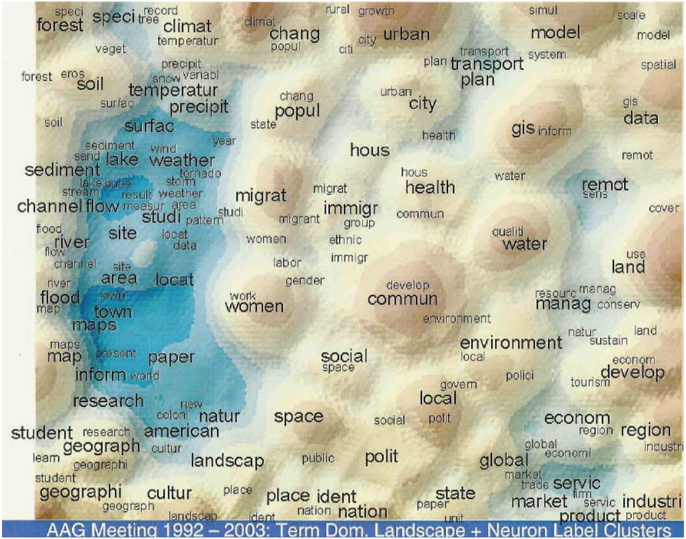
Clustering topical areas

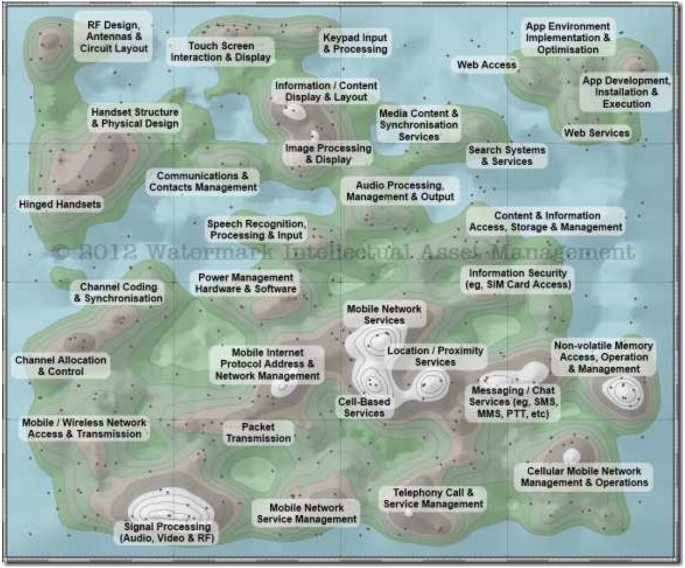


Clustering what appears in AAG conferences

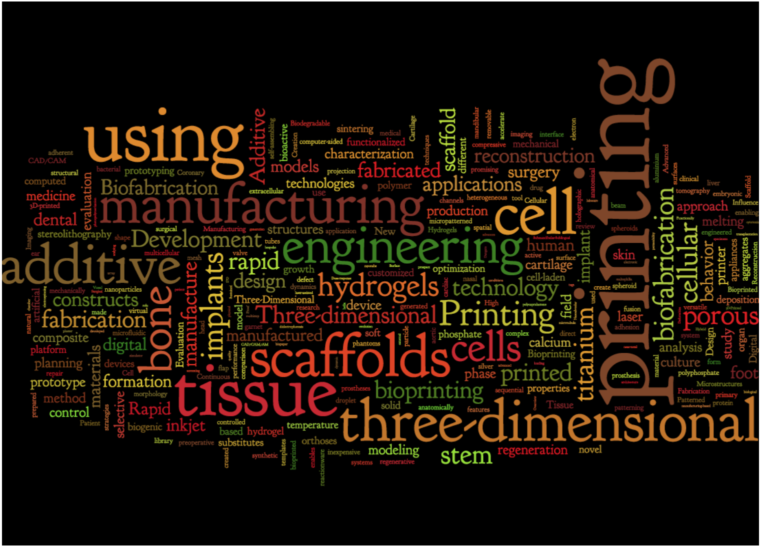


(AAG = Association of American Geographers)

Clustering patents


RF Design, Antennas & Circuit Layout
Touch Screen Interaction & Display
Keypad Input & Processing
App Environment Implementation & Optimisation
Web Access
App Development, Installation & Execution
Information / Content Display & Layout
Handset Structure & Physical Design
Media Content & Synchronisation Services
Web Services
Image Processing & Display
Search Systems & Services
Communications & Contacts Management
Audio Processing, Management & Output
Hinged Handsets
Content & Information Access, Storage & Management
Speech Recognition, Processing & Input
© 2012 Watermark Intellectual Asset Management
Power Management Hardware & Software
Information Security (eg, SIM Card Access)
Channel Coding & Synchronisation
Mobile Network Services
Location / Proximity Services
Non-volatile Memory Access, Operation & Management
Channel Allocation & Control
Mobile Internet Protocol Address & Network Management
Messaging / Chat Services (eg, SMS, MMS, PTT, etc)
Cell-Based Services
Mobile / Wireless Network Access & Transmission
Packet Transmission
Cellular Mobile Network Management & Operations
Telephony Call & Service Management
Mobile Network Service Management
Signal Processing (Audio, Video & RF)

Clustering terms



Types of Clustering

- Hard clustering v. soft clustering
  - Hard clustering: every object is member in only one cluster
  - Soft clustering: objects can be members in more than one cluster
- Hierarchical v. non-hierarchical clustering
  - Hierarchical clustering: pairs of most-similar clusters are iteratively linked until all objects are in a clustering relationship
  - Non-hierarchical clustering results in flat clusters of “similar” documents

Desiderata for clustering

- General goal: put related docs in the same cluster, put unrelated docs in different clusters.
  - We'll see different ways of formalizing this.
- The number of clusters should be appropriate for the data set we are clustering.
  - Initially, we will assume the number of clusters K is given.
  - There also exist semiautomatic methods for determining K
- Secondary goals in clustering
  - Avoid very small and very large clusters
  - Define clusters that are easy to explain to the user
  - Many others . . .

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Non-hierarchical (partitioning) clustering

- Partitional clustering algorithms produce a set of k non-nested partitions corresponding to k clusters of n objects.
- Advantage: not necessary to compare each object to each other object, just comparisons of objects – cluster centroids necessary
- Optimal partitioning clustering algorithms are $O(kn)$
- Main algorithm: K-means

K-means: Basic idea

- Each cluster j (with n_j elements x_i) is represented by its centroid c_j, the average vector of the cluster:

$$c_j = \frac{1}{n_j} \sum_{i=1}^{n_j} x_i$$

- Measure of cluster quality: minimise mean square distance between elements x_i and nearest centroid c_j

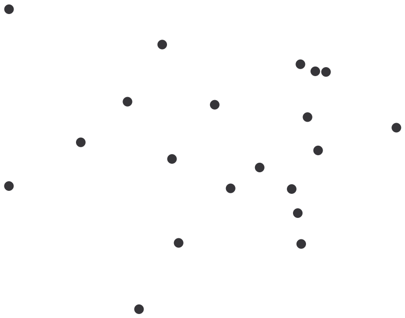
$$RSS = \sum_{j=1}^{k} \sum_{x_i \in j} d(\vec{x_i}, \vec{c_j})^2$$

- Distance: Euclidean; length-normalised vectors in VS
- We iterate two steps:
  - reassignment: assign each vector to its closest centroid
  - recomputation: recompute each centroid as the average of the vectors that were recently assigned to it

K-means algorithm

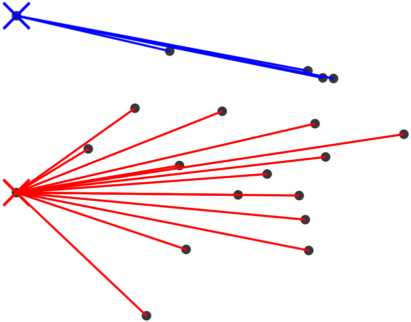
```
Given: a set $s_0 = \overrightarrow{x_1}, ...\overrightarrow{x_n} \subseteq \mathcal{R}^m$
Given: a distance measure $d : \mathcal{R}^m \times \mathcal{R}^m \rightarrow \mathcal{R}$
Given: a function for computing the mean $\mu : \mathcal{P}(\mathcal{R}) \rightarrow \mathcal{R}^m$

Select $k$ initial centers $\overrightarrow{c_1}, ...\overrightarrow{c_k}$
while stopping criterion not true:
        $\sum_{j=1}^{k} \sum_{x_i \in s_j} d(\overrightarrow{x_i}, \overrightarrow{c_j})^2 < \epsilon$ (stopping criterion)
        do
        for all clusters $s_j$ do (reassignment)
                $c_j := \{\overrightarrow{x_i} | \forall \overrightarrow{c_l} : d(\overrightarrow{x_i}, \overrightarrow{c_j}) \leq d(\overrightarrow{x_i}, \overrightarrow{c_l})\}$
        end
        for all means $\overrightarrow{c_j}$ do (centroid recomputation)
                $\overrightarrow{c_j} := \mu(s_j)$
        end
end
```

Worked Example: Set of points to be clustered



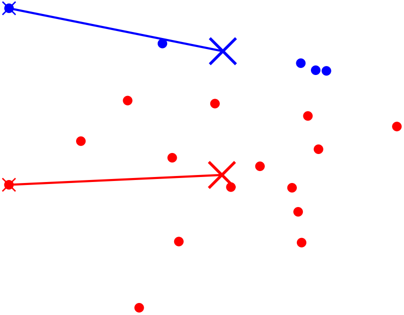
Exercise: (i) Guess what the optimal clustering into two clusters is in this case; (ii) compute the centroids of the clusters

Random seeds + Assign points to closest center



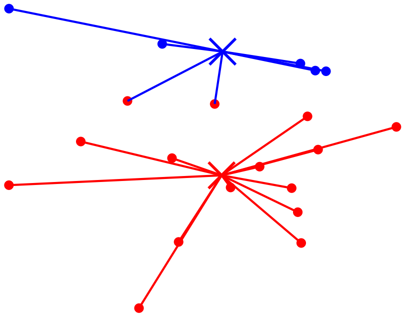
Iteration One

Worked Example: Recompute cluster centroids



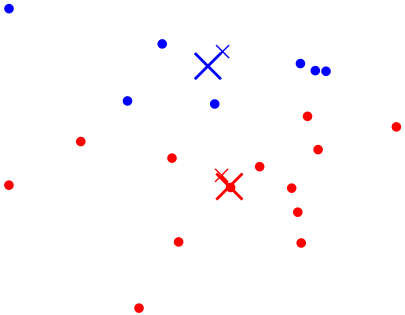
Iteration One

Worked Example: Assign points to closest centroid



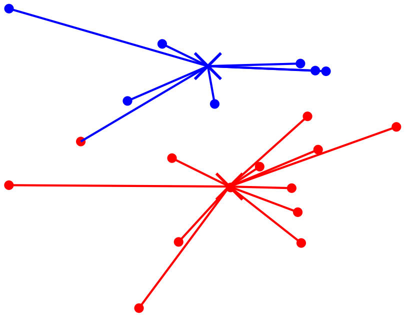
Iteration One

Worked Example: Recompute cluster centroids



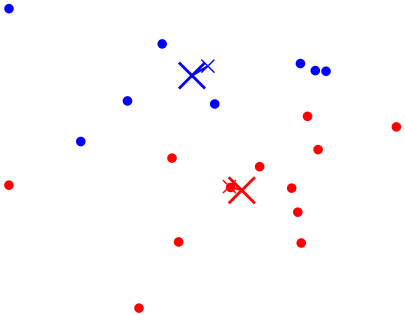
Iteration Two

Worked Example: Assign points to closest centroid



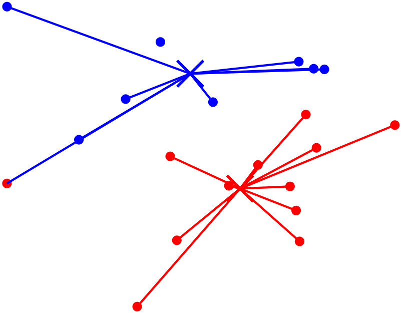
Iteration Two

Worked Example: Recompute cluster centroids



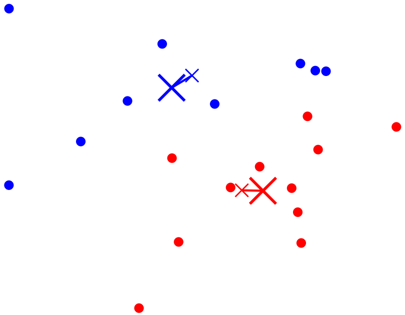
Iteration Three

Worked Example: Assign points to closest centroid



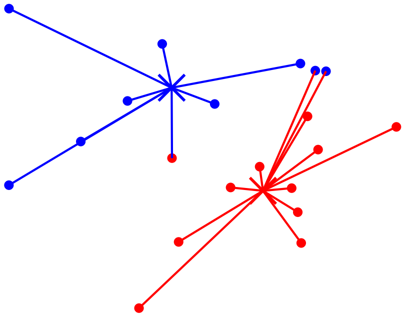
Iteration Three

Worked Example: Recompute cluster centroids



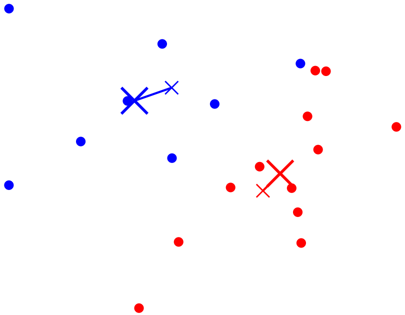
Iteration Four

Worked Example: Assign points to closest centroid



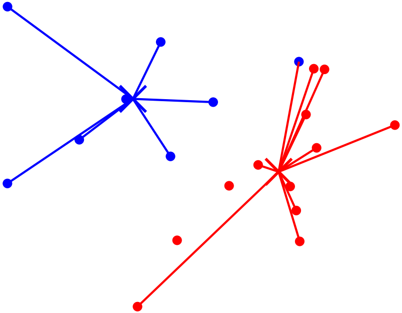
Iteration Four

Worked Example: Recompute cluster centroids



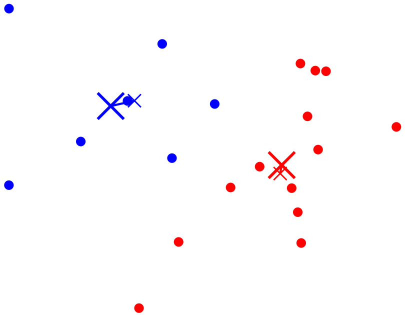
Iteration Five

Worked Example: Assign points to closest centroid



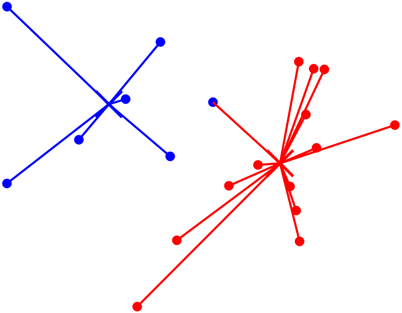
Iteration Five

Worked Example: Recompute cluster centroids



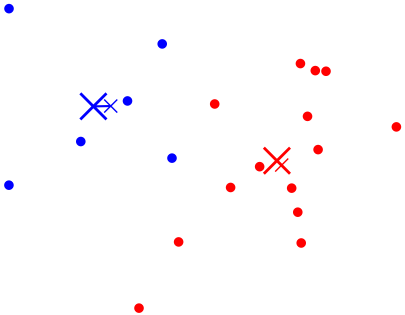
Iteration Six

Worked Example: Assign points to closest centroid



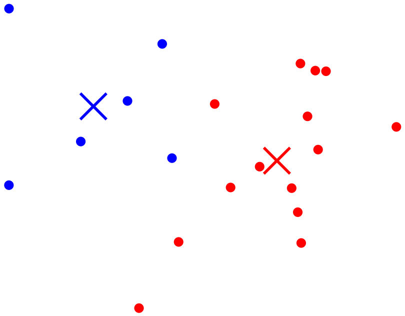
Iteration Six

Worked Example: Recompute cluster centroids



Iteration Seven

Worked Ex.: Centroids and assignments after convergence



Convergence

K-means is guaranteed to converge: Proof

- RSS decreases during each reassignment step.
  - because each vector is moved to a closer centroid
- RSS decreases during each recomputation step.
  - This follows from the definition of a centroid: the new centroid is the vector for which RSS_k reaches its minimum
- There is only a finite number of clusterings.
- Thus: We must reach a fixed point.
- Finite set & monotonically decreasing evaluation function → convergence
- Assumption: Ties are broken consistently.

Other properties of K-means

- Fast convergence
  - K-means typically converges in around 10-20 iterations (if we don't care about a few documents switching back and forth)
  - However, complete convergence can take many more iterations.
- Non-optimality
  - K-means is not guaranteed to find the optimal solution.
  - If we start with a bad set of seeds, the resulting clustering can be horrible.
- Dependence on initial centroids
  - Solution 1: Use i clusterings, choose one with lowest RSS
  - Solution 2: Use prior hierarchical clustering step to find seeds with good coverage of document space

Time complexity of K-means

- Reassignment step: $O(KNM)$ (we need to compute KN document-centroid distances, each of which costs $O(M)$
- Recomputation step: $O(NM)$ (we need to add each of the document's $< M$ values to one of the centroids)
- Assume number of iterations bounded by I
- Overall complexity: $O(IKNM)$ – linear in all important dimensions

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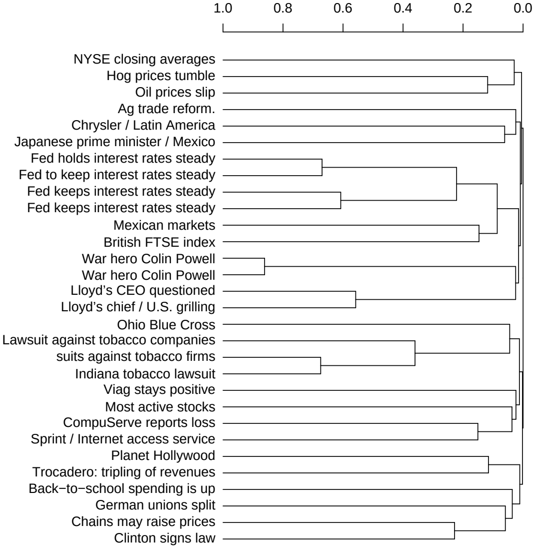
Hierarchical clustering

- Imagine we now want to create a hierachy in the form of a binary tree.
- Assumes a similarity measure for determining the similarity of two clusters.
- Up to now, our similarity measures were for documents.
- We will look at different cluster similarity measures.
- Main algorithm: HAC (hierarchical agglomerative clustering)

HAC: Basic algorithm

- Start with each document in a separate cluster
- Then repeatedly merge the two clusters that are most similar
- Until there is only one cluster.
- The history of merging is a hierarchy in the form of a binary tree.
- The standard way of depicting this history is a dendrogram.

A dendrogram



Term–document matrix to document–document matrix

Log frequency weighting
and cosine normalisation

SaS	PaP	WH
0.789	0.832	0.524
0.515	0.555	0.465
0.335	0.000	0.405
0.000	0.000	0.588

SaS	P(SaS,SaS)	P(PaP,SaS)
PaP	P(SaS,PaP)	P(PaP,PaP)
WH	P(SaS,WH)	P(PaP,WH)
	SaS	PaP

SaS	1	.94	.79
PaP	.94	1	.69
WH	.79	.69	1
	SaS	PaP	WH

- Applying the proximity metric to all pairs of documents...
- creates the document-document matrix, which reports similarities/distances between objects (documents)
- The diagonal is trivial (identity)
- As proximity measures are symmetric, the matrix is a triangle

Hierarchical clustering: agglomerative (BottomUp, greedy)

```
Given: a set $X = x_1, ...x_n$ of objects;
Given: a function $sim : \mathcal{P}(X) \times \mathcal{P}(X) \rightarrow \mathcal{R}$

for i:= 1 to n do
        $c_i := x_i$
C :=$c_1$, ... $c_n$
j := n+1
while C > 1 do
        $(c_{n_1}, c_{n_2}) := max_{(c_u, c_v) \in C \times C} sim(c_u, c_v)$
        $c_j := c_{n_1} \cup c_{n_2}$
        C := C  $\{ c_{n_1}, c_{n_2} \} \cup c_j$
        j:=j+1
end
```

Similarity function $sim : \mathcal{P}(X) \times \mathcal{P}(X) \rightarrow \mathcal{R}$ measures similarity between clusters, not objects

Computational complexity of the basic algorithm

- First, we compute the similarity of all $N \times N$ pairs of documents.
- Then, in each of N iterations:
  - We scan the $O(N \times N)$ similarities to find the maximum similarity.
  - We merge the two clusters with maximum similarity.
  - We compute the similarity of the new cluster with all other (surviving) clusters.
- There are $O(N)$ iterations, each performing a $O(N \times N)$ "scan" operation.
- Overall complexity is $O(N^3)$.
- Depending on the similarity function, a more efficient algorithm is possible.

Hierarchical clustering: similarity functions

Similarity between two clusters c_k and c_j (with similarity measure s) can be interpreted in different ways:

- Single Link Function: Similarity of two most similar members

  $$sim(c_u, c_v) = max_{x \in c_u, y \in c_k} s(x, y)$$

- Complete Link Function: Similarity of two least similar members

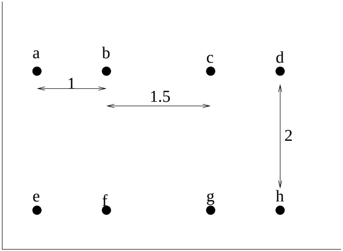
  $$sim(c_u, c_v) = min_{x \in c_u, y \in c_k} s(x, y)$$

- Group Average Function: Avg. similarity of each pair of group members

  $$sim(c_u, c_v) = avg_{x \in c_u, y \in c_k} s(x, y)$$

Example: hierarchical clustering; similarity functions

Cluster 8 objects a-h; Euclidean distances (2D) shown in diagram



b	1						
c	2.5	1.5					
d	3.5	2.5	1				
e	2	$\sqrt{5}$	$\sqrt{10.25}$	$\sqrt{16.25}$			
f	$\sqrt{5}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$	1		
g	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\sqrt{5}$	2.5	1.5	
h	$\sqrt{16.25}$	$\sqrt{10.25}$	$\sqrt{5}$	2	3.5	2.5	1
	a	b	c	d	e	f	g

Single Link is O(n^2)

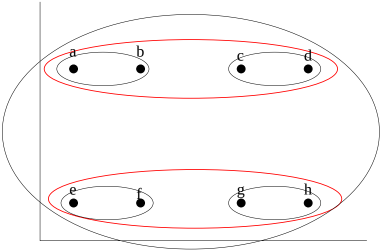
b	1						
c	2.5	1.5					
d	3.5	2.5	1				
e	2	$\sqrt{5}$	$\sqrt{10.25}$	$\sqrt{16.25}$			
f	$\sqrt{5}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$	1		
g	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\sqrt{5}$	2.5	1.5	
h	$\sqrt{16.25}$	$\sqrt{10.25}$	$\sqrt{5}$	2	3.5	2.5	1
	a	b	c	d	e	f	g

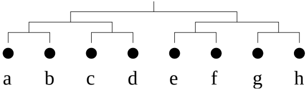
After Step 4 (a–b, c–d, e–f, g–h merged):

c–d	1.5		
e–f	2	$\sqrt{6.25}$	
g–h	$\sqrt{6.25}$	2	1.5
	a–b	c–d	e–f

"min-min" at each step

Clustering Result under Single Link





Complete Link

b	1						
c	2.5	1.5					
d	3.5	2.5	1				
e	2	$\sqrt{5}$	$\sqrt{10.25}$	$\sqrt{16.25}$			
f	$\sqrt{5}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$	1		
g	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\sqrt{5}$	2.5	1.5	
h	$\sqrt{16.25}$	$\sqrt{10.25}$	$\sqrt{5}$	2	3.5	2.5	1
	a	b	c	d	e	f	g

After step 4 (a–b, c–d, e–f, g–h merged):

c–d	2.5 1.5 $\boxed{3.5}$ 2.5		
e–f	2 $\sqrt{5}$ $\boxed{\sqrt{5}}$ 2	$\sqrt{10.25}$ $\boxed{\sqrt{16.25}}$ $\sqrt{6.25}$ $\sqrt{10.25}$	
g–h	$\sqrt{10.25}$ $\sqrt{6.25}$ $\boxed{\sqrt{16.25}}$ $\sqrt{10.25}$	2 $\boxed{\sqrt{5}}$ $\sqrt{5}$ 2	2.5 1.5 $\boxed{3.5}$ 2.5
	a–b	c–d	e–f

"max-min" at each step

Complete Link

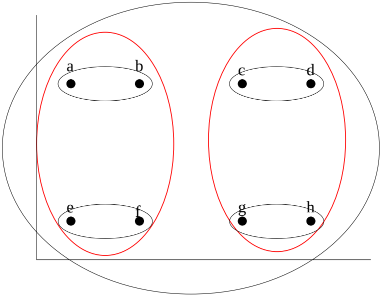
b	1						
c	2.5	1.5					
d	3.5	2.5	1				
e	2	$\sqrt{5}$	$\sqrt{10.25}$	$\sqrt{16.25}$			
f	$\sqrt{5}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$	1		
g	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\sqrt{5}$	2.5	1.5	
h	$\sqrt{16.25}$	$\sqrt{10.25}$	$\sqrt{5}$	2	3.5	2.5	1
	a	b	c	d	e	f	g

After step 4 (a–b, c–d, e–f, g–h merged):

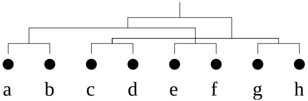
c–d	2.5	1.5				
	$\boxed{3.5}$	2.5				
e–f	2	$\sqrt{5}$	$\sqrt{10.25}$	$\boxed{\sqrt{16.25}}$		
	$\boxed{\sqrt{5}}$	2	$\sqrt{6.25}$	$\sqrt{10.25}$		
g–h	$\sqrt{10.25}$	$\sqrt{6.25}$	2	$\boxed{\sqrt{5}}$	2.5	1.5
	$\boxed{\sqrt{16.25}}$	$\sqrt{10.25}$	$\sqrt{5}$	2	$\boxed{3.5}$	2.5
	a–b		c–d		e–f	

“max-min” at each step → ab/ef and cd/gh merges next

Clustering result under complete link



Complete Link is $O(n^3)$



Example: gene expression data

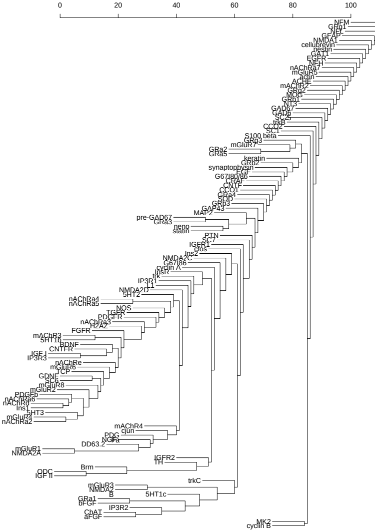
- An example from biology: cluster genes by function
- Survey 112 rat genes which are suspected to participate in development of CNS
- Take 9 data points: 5 embryonic (E11, E13, E15, E18, E21), 3 postnatal (P0, P7, P14) and one adult
- Measure expression of gene (how much mRNA in cell?)
- These measures are normalised logs; for our purposes, we can consider them as weights
- Cluster analysis determines which genes operate at the same time

Rat CNS gene expression data (excerpt)

gene	genbank locus	E11	E13	E15	E18	E21	P0	P7	P14	A
keratin	RNKER19	1.703	0.349	0.523	0.408	0.683	0.461	0.32	0.081	0
cellubrevin	s63830	5.759	4.41	1.195	2.134	2.306	2.539	3.892	3.953	2.72
nestin	RATNESTIN	2.537	3.279	5.202	2.807	1.5	1.12	0.532	0.514	0.443
MAP2	RATMAP2	0.04	0.514	1.553	1.654	1.66	1.491	1.436	1.585	1.894
GAP43	RATGAP43	0.874	1.494	1.677	1.937	2.322	2.296	1.86	1.873	2.396
L1	S55536	0.062	0.162	0.51	0.929	0.966	0.867	0.493	0.401	0.384
NFL	RATNFL	0.485	5.598	6.717	9.843	9.78	13.466	14.921	7.862	4.484
NFM	RATNFM	0.571	3.373	5.155	4.092	4.542	7.03	6.682	13.591	27.692
NFH	RATNFHPEP	0.166	0.141	0.545	1.141	1.553	1.667	1.929	4.058	3.859
synaptophysin	RNSYN	0.205	0.636	1.571	1.476	1.948	2.005	2.381	2.191	1.757
neno	RATENONS	0.27	0.704	1.419	1.469	1.861	1.556	1.639	1.586	1.512
S100 beta	RATS100B	0.052	0.011	0.491	1.303	1.487	1.357	1.438	2.275	2.169
GFAP	RNU03700	0	0	0	0.292	2.705	3.731	8.705	7.453	6.547
MOG	RATMOG	0	0	0	0	0.012	0.385	1.462	2.08	1.816
GAD65	RATGAD65	0.353	1.117	2.539	3.808	3.212	2.792	2.671	2.327	2.351
pre-GAD67	RATGAD67	0.073	0.18	1.171	1.436	1.443	1.383	1.164	1.003	0.985
GAD67	RATGAD67	0.297	0.307	1.066	2.796	3.572	3.182	2.604	2.307	2.079
G67I80/86	RATGAD67	0.767	1.38	2.35	1.88	1.332	1.002	0.668	0.567	0.304
G67I86	RATGAD67	0.071	0.204	0.641	0.764	0.406	0.202	0.052	0.022	0
GAT1	RATGABAT	0.839	1.071	5.687	3.864	4.786	4.701	4.879	4.601	4.679
ChAT	(*)	0	0.022	0.369	0.322	0.663	0.597	0.795	1.015	1.424
ACHE	S50879	0.174	0.425	1.63	2.724	3.279	3.519	4.21	3.885	3.95
ODC	RATODC	1.843	2.003	1.803	1.618	1.569	1.565	1.394	1.314	1.11
TH	RATTOHA	0.633	1.225	1.007	0.801	0.654	0.691	0.23	0.287	0
NOS	RRBNOS	0.051	0.141	0.675	0.63	0.86	0.926	0.792	0.646	0.448
GRa1	(#)	0.454	0.626	0.802	0.972	1.021	1.182	1.297	1.469	1.511

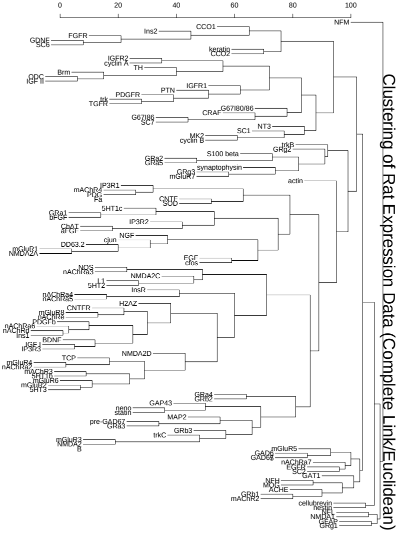
...

Rat CNS gene clustering – single link

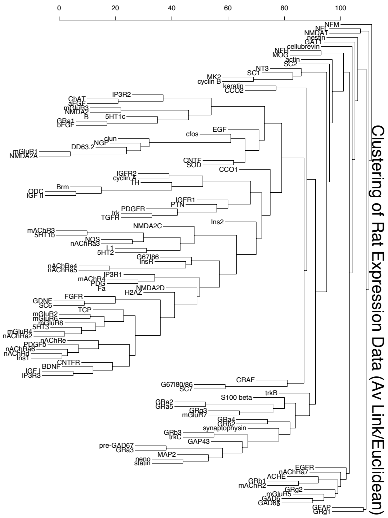


Clustering of Rat Expression Data (Single Link/Euclidean)

Rat CNS gene clustering – complete link



Rat CNS gene clustering – group average link



Flat or hierarchical clustering?

- When a hierarchical structure is desired: hierarchical algorithm
- Humans are bad at interpreting hiearchical clusterings (unless cleverly visualised)
- For high efficiency, use flat clustering
- For deterministic results, use HAC
- HAC also can be applied if K cannot be predetermined (can start without knowing K)

Take-away

- Partitional clustering
  - Provides less information but is more efficient (best: $O(kn)$)
  - K-means
- Hierarchical clustering
  - Best algorithms $O(n^2)$ complexity
  - Single-link vs. complete-link (vs. group-average)
- Hierarchical and non-hierarchical clustering fulfills different needs

Reading

- MRS Chapters 16.1-16.4
- MRS Chapters 17.1-17.2